

Comment on “Numerical estimates of the spectrum for anharmonic \mathcal{PT} symmetric potentials” by Bowen *et al*

Carl M. Bender¹ and Stefan Boettcher²

¹*Department of Physics, Washington University, St. Louis, MO 63130, USA*

²*Department of Physics, Emory University, Atlanta, GA 30322, USA*

(Dated: October 2, 2012)

The paper by Bowen, Mancini, Fessatidis, and Murawski (2012 Phys. Scr. **85**, 065005) demonstrates in a dramatic fashion the serious difficulties that can arise when one rushes to perform numerical studies before understanding the physics and mathematics of the problem at hand and without understanding the limitations of the numerical methods used. Based on their flawed numerical work, the authors conclude that the work of Bender and Boettcher is wrong even though it has been verified at a completely rigorous level. Unfortunately, the numerical procedures performed and described in the paper by Bowen *et al* are incorrectly applied and wrongly interpreted.

PACS numbers: 11.15.Pg, 11.30.Er, 03.65.Db

The key sentence in the paper by Bowen *et al* [1] is in Section 3 (Discussion): “The mystery of this study is why does this numerical method give such radically different results from those discussed by Bender.” As we explain in the present Comment, the simple and straightforward explanation of this “mystery” is that the results reported in Bender and Boettcher [2] are correct and that the numerical work reported in the paper by Bowen *et al* is incorrect and misinterpreted.

In the original paper by Bender and Boettcher [2], the eigenvalues of the \mathcal{PT} -symmetric Hamiltonian

$$H = p^2 + x^2(ix)^\varepsilon, \quad (1)$$

where ε is a real parameter, were studied in great detail by using both numerical and perturbative methods. It was shown that when $\varepsilon \geq 0$, the eigenvalues are real, positive, and discrete and that there are no complex eigenvalues. These conclusions were subsequently verified in rigorous studies by Dorey, Dunning, and Tateo [3] and Shin [4].

Before one can perform numerical calculations of the eigenvalues of the Hamiltonian (1), it is essential to understand what it means to extend an eigenvalue problem into the complex domain. The first detailed work in this area was done by Bender and Wu [5], who examined the behavior of the eigenvalues of the quartic anharmonic oscillator as functions of complex coupling constant. Further studies of analytically continued eigenvalue problems were done by Bender and Turbiner [6]. The crucial element explained in all of these studies is that as a parameter in an eigenvalue differential equation is varied, the Stokes wedges in which the boundary conditions on the eigenfunctions are imposed must rotate as functions of that parameter.

To be specific, the eigenvalues associated with the Hamiltonian (1) are determined by the complex differential equation

$$-\psi''(x) + x^2(ix)^\varepsilon\psi(x) = E\psi(x) \quad (2)$$

and a pair of \mathcal{PT} -symmetric boundary conditions in the complex- x plane: $\psi(x) \rightarrow 0$ as $|x| \rightarrow \infty$ with $\arg x$ lying inside the opening angles of the Stokes wedges.

The details of how to find the opening angles of Stokes wedges are not given here because detailed explanations are given in Refs. [2, 7, 8]. We simply state the results: When $\varepsilon = 0$, the two Stokes wedges have opening angles of 90° and are centered about the positive-real and negative-real axes. As ε increases from 0, the Stokes wedges become thinner and rotate downward into the lower-half complex- x plane. When ε reaches the value 2, the opening angles of the wedges have decreased to 60° and the wedges no longer contain the positive- and negative-real axes.

Because the eigenvalue differential equation (2) must be solved along a contour in the complex- x plane that terminates in the Stokes wedges, it is best to solve the differential equation numerically on a complex contour by using the standard Runge-Kutta method. The Runge-Kutta procedure described in Refs. [2, 6] has the obvious advantage that it can be used for any real value of ε , and not just for integer ε . It is also extremely important to understand that different pairs of Stokes wedges give different sets of eigenvalues. For example, for the quantum harmonic oscillator Hamiltonian $H = p^2 + x^2$, which corresponds to $\varepsilon = 0$ in (1), if Stokes wedges containing the real axes are used, the eigenvalues are 1, 3, 5, 7, ..., which are strictly positive. However, if Stokes wedges containing the imaginary axes are used, the eigenvalues are $-1, -3, -5, -7, \dots$, which are strictly negative.

In the paper by Bowen *et al* a clumsy and inappropriate numerical procedure for calculating the eigenvalues is used in which the Hamiltonian is expanded in terms of Harmonic-oscillator basis functions. The procedure is clumsy because the algebra becomes much too unwieldy when ε is noninteger. Thus, in the paper by Bowen *et al* the procedure was limited to the very special cases $\varepsilon = 0, 1, 2, 4, 6$.

Furthermore, while the harmonic-oscillator eigenfunctions are complete on the real axis, *these basis functions*

are not complete in the complex plane, so these basis functions cannot be used unless the Stokes wedges include the real axis.[9] Thus, the numerical calculations that were performed by Bowen *et al* are completely invalid and meaningless except for the trivial case of the harmonic-oscillator ($\varepsilon = 0$) and the more interesting and nontrivial case $\varepsilon = 1$.

Unfortunately, Bowen *et al* made a long sequence of wrong arguments and completely misinterpreted the numerical results that they obtained for the $\varepsilon = 1$ case. While it is perfectly correct to expand $H = p^2 + ix^3$ in an *infinite* harmonic-oscillator basis, Bowen *et al* then truncate the infinite matrix representation of the Hamiltonian, which is \mathcal{PT} symmetric, to an $N \times N$ matrix, which is no longer \mathcal{PT} symmetric. As a result, the finite-dimensional matrix has complex eigenvalues. These complex eigenvalues reported by Bowen *et al* are merely artifacts of the truncation procedure that they used.

Bowen *et al* then go on to make further serious misjudgments. The procedure of truncating an infinite matrix is *variational* in character. Thus, it can only be used to compute the low-lying eigenvalues. If the procedure is used carefully and properly, one follows the behavior of the low-lying eigenvalues as N increases and observes that at first the behavior is irregular and complex. (The behavior of the eigenvalues is not monotone because the $N \times N$ matrix is not Hermitian.) However, as N gets larger, one observes that the eigenvalues settle down

one-by-one starting at the low-energy end of the spectrum, and stabilize at the real values found by Bender and Boettcher. This stabilization process is extremely slow; for very large N , say 100, only about half a dozen eigenvalues can be determined with any useful accuracy. The rest of the eigenvalues of the $N \times N$ matrix bear no resemblance to the true eigenvalues of the Hamiltonian $H = p^2 + ix^3$. Unfortunately, Bowen *et al* take their numerical results for the high-lying eigenvalues seriously in their paper even though they have no numerical accuracy whatsoever. Indeed for the $p^2 + ix^3$ Hamiltonian, WKB predicts that the n th eigenvalue grows like $n^{6/5}$ for large n , whereas the numerical work of Bowen *et al* gives nothing of the sort.

Before concluding, we point out that Bowen *et al* could have benefited by actually reading and understanding the review paper Ref. [7]. They clearly did not do so because no less than five times in their six-page paper they make the ridiculous claim that in this review paper Bender states that the Hamiltonian $H = p^2 - x^2$ has real, discrete, negative eigenvalues. In fact, this Hamiltonian certainly does not have real negative eigenvalues, and Bender has never made such an absurd claim in any paper.

CMB is supported by the U.S. Department of Energy and SB is supported by U.S. National Science Foundation.

-
- [1] Bowen S P, Mancini J D, Fessatidis V, and Murawski R K, 2012 *Phys. Scr.* **85**, 065005
 - [2] Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **80**, 5243
 - [3] Dorey P, Dunning C, and Tateo R 2001 *J. Phys. A: Math. Gen.* **34**, 5679; (2004) *Czech. J. Phys.* **54**, 35
 - [4] Shin K C, 2001 *J. Math. Phys.* **42**, 2513; 2002 *Commun. Math. Phys.* **229**, 543; 2004 *J. Phys. A: Math. Gen.* **37**, 8287
 - [5] Bender C M and Wu T T 1969 *Phys. Rev.* **184**, 1231
 - [6] Bender C M and Turbiner A 1993 *Phys. Lett. A* **173**, 442
 - [7] Bender C M 2007 *Rep. Prog. Phys.* **70**, 947
 - [8] C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978), Chap. 6.
 - [9] One has exactly the same problem with the sine and cosine functions that are used to construct Fourier series. These trigonometric functions form a complete basis on a portion of the real axis, but these functions are definitely not complete in the complex plane.